

Shaking during Ion-Atom Collisions

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Abstract

Shaking (shakeup + shakeoff) probabilities accompanying ion-atom collisions are studied using hydrogenic wavefunctions for K-, L-, M- shell electrons in the sudden approximation limit. The role of recoil velocity in the shaking processes is discussed. Further, it is found that the suddenness of collision between projectile and target nuclei plays a major factor in shaking of respective atomic system than the recoil of nuclei.

Keywords: Ion-atom collision, Electronic excitation & ionization, Shaking process, Sudden approximation, Hydrogenic wavefunction

1. Introduction

All nuclear and atomic events result in a change in the central potential and/or electronic environment of the corresponding atomic system. If the perturbation or net change in system occurs suddenly enough, then the orbital
 5 electrons may not respond so rapidly to rearrange themselves. This process subsequently leads to the electrons getting excited to an unoccupied bound state (shakeup process) or leaving the parent atom/ion (shakeoff process). This process is called shaking process [1]. Theoretically shaking processes are treated under the sudden approximation limit [2]. It is worth to note that a perturbation
 10 tion is called sudden if the time period τ of perturbation is less than that of periodic motion, $2\pi\omega_n^{-1}$, of the orbital electrons [3]. There are many nuclear

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processes e.g. β -decay [4, 5], α -transfer reactions [6], positron decay [7], internal conversion [8, 9] as well as atomic processes e.g. photoionization [10], inner-shell ionization [11], orbital electron capture [12, 13] etc. in which the condition of suddenness satisfies. In a similar phenomenon, if the nuclei receives a sudden jolt in its normal state, it may lead to the ionization or excitation of electrons in the atomic system. During fast ion-atom collisions target or projectile nuclei receives similar type of sudden jolt which can result in sudden change of the position of respective nuclei and thus creates a sudden perturbation in atomic electronic configuration to initiate the shaking processes. The sudden perturbation in electronic environment solely depends on the recoil of the target atom or incident projectile ion and therefore it affects also the projectile ion in same manner as target atom. The basic formulation to calculate shaking probability under the sudden jolt of nuclei is described in the book by Landau and Lifshitz [14] using nonrelativistic hydrogenic wave functions. But the work is only limited to the hydrogen atom. The present work is an extension of the previous work to define the general expression for shaking probability for K-, L- and M- shell electrons of any atom using the hydrogenic wavefunctions due to the sudden jolt of nuclei during ion-atom collisions.

2. Formalism of the Shaking Process

Basically, shaking is a two-step process, in the first step due to the sudden perturbation, the central potential of parent atomic system or electronic environment gets disturbed, whereas in the second step under such influence electrons make transition to a new state (shakeup) or continuum state (shake-off). In the case of ion-atom collisions, first step corresponds to sudden impact of projectile nuclei to target nuclei and second step resembles the shaking of electrons due to recoil of respective nuclei. Worth to note that, shaking due to sudden jolt of nuclei strongly depends on the first step or the amplitude of ion-atom impact, whereas shaking due to other processes e.g. inner shell ionization [11], photoionization [10] etc. does not depend on the physical nature of first

step.

The shaking probability of the system from one state to another due to sudden jolt can be determined from the general quantum mechanics rules, by the overlap integral of the corresponding wave functions [14, 15, 16]

$$W_{fi} = \left| \int \psi_f^* \psi_i^{(0)} dq \right|^2 \quad (1)$$

45 The both wave functions $\psi_i^{(0)}$ and ψ_f are stationary and related to the Hamiltonians \hat{H}_0 and \hat{H} , respectively. Due to the stationary nature, the wavefunctions associated with the probability density is independent of time and have the form $\Psi = \psi(q) \exp(-iEt/\hbar)$, where the wave function depends only on the position coordinates and independent of the energy. As a result of the suddenness of
50 perturbation, the electronic wave function of the system "has no time" to change from initial to final state and therefore remains intact as they were before the perturbation. Therefore they will no longer represent the characteristic wave functions of the new Hamiltonian of the system and will not corresponds the stationary states. In another words, shaking phenomena is the imperfect overlap
55 of the initial and final electronic wave functions. For the case of non-relativistic hydrogenic wavefunctions Eq. 1 can be rewritten as

$$W_{fi} = \left| \int \psi_{n'l'm'}^* \psi_{nlm} dq \right|^2 \quad (2)$$

where n, l, m and n', l', m' are the quantum numbers of the initial and final atomic system, respectively. Important to note that, since the shake process has a monopole character, the selection rule for shaking processes only favours such
60 transitions in which the principal quantum number of the final state is different from the initial i.e. $n' \neq n$ and all other quantum numbers remain same i.e. $l' = l$ and $m' = m$. Thus the Eq. 2 can be simplified to

$$W_{fi} = \left| \int \psi_{n'l'm}^* \psi_{nlm} dq \right|^2 \quad (3)$$

3. Theoretical work, Results and Discussion

Total shaking probability of target atom or projectile ion due to the ion-atom collision can be calculated using the Eq. 3. Normalized wave functions corresponding to K-, L- and M- shells for an "infinitely heavy nucleus" [17] given in Table 1 are used to calculate the integral of Eq. 3.

It is worth to mention that after the sudden change occurring in the central potential or electronic environment, each electron has three possibilities in the new environment. It may remain either in the same state or can make a transition to unoccupied bound state (shakeup) or gets ionized to the continuum state (shakeoff). It is already mentioned in previous section that shaking of atom/ion is the sum of shakeup and shakeoff processes. So better way to calculate shaking probability is to subtract the probability that all the electron will remain in their initial state from the total probability i.e. unity. This method was applied by the earlier workers [11, 18] to calculate the shaking probabilities following the inner-shell vacancy production.

Now, during the ion-atom collisions the nucleus of the target atom/ projectile ion receives an impact which gives it a recoil velocity v . If this perturbation i.e. impact is sudden relative to electron orbital periods, it can lead to the excitation or ionization of the electrons [14]. Now, let us first discuss about sudden jolt in the target nuclei, assuming lab frame of reference is S . After the ion-atom collision the frame of reference is S' , which is moving with the nucleus. Due to the suddenness of perturbation the coordinates of electrons in S' are same as S . The initial wave function of electron in S' is given by

$$\psi'_0 = \psi_0 \exp \left(-iq \cdot \sum_p r_p \right) \quad (4)$$

Here, $q = mv/\hbar$, v = atom/ion recoil velocity, m = atom/ion mass, summation is over all Z electrons in the atom and ψ_0 is the wave function of electron when the nucleus is at rest or in frame S .

From the Eq. 3, the required probability of electron to remain in the same

Table 1: Normalized non-relativistic hydrogenic wave functions (in real forms) corresponding to the first three shells K-, L- and M- shells electrons. The spectroscopic notation s have their usual meanings.

Shell	Quantum Numbers	Spectroscopic Notation	Wavefunction $\psi_{nlm}(r, \theta, \phi)$
K	1 0 0	1s	$\frac{1}{\sqrt{\pi}} \left(\frac{Z}{a}\right)^{3/2} \exp\left(-\frac{Zr}{a}\right)$
L	2 0 0	2s	$\frac{1}{2\sqrt{2\pi}} \left(\frac{Z}{a}\right)^{3/2} \left(1 - \frac{Zr}{2a}\right) \exp\left(-\frac{Zr}{2a}\right)$
	2 1 0	2p _z	$\frac{1}{4\sqrt{2\pi}a} \left(\frac{Z}{a}\right)^{3/2} \frac{Zr}{a} \exp\left(-\frac{Zr}{2a}\right) \cos \theta$
	2 1 1	2p _y	$\frac{1}{8\sqrt{\pi}} \left(\frac{Z}{a}\right)^{3/2} \frac{Zr}{a} \exp\left(-\frac{Zr}{2a}\right) \sin \theta \cos \phi$
	2 1 -1	2p _x	$\frac{1}{8\sqrt{\pi}} \left(\frac{Z}{a}\right)^{3/2} \frac{Zr}{a} \exp\left(-\frac{Zr}{2a}\right) \sin \theta \sin \phi$
M	3 0 0	3s	$\frac{1}{3\sqrt{3\pi}} \left(\frac{Z}{a}\right)^{3/2} \left(\frac{2r^2 Z^2}{27a^2} - \frac{2Zr}{3a} + 1\right) \exp\left(-\frac{Zr}{3a}\right)$
	3 1 0	3p _z	$\frac{2\sqrt{2}}{27\sqrt{\pi}} \left(\frac{Z}{a}\right)^{3/2} \frac{Zr}{a} \left(1 - \frac{Zr}{6a}\right) \exp\left(-\frac{Zr}{3a}\right) \cos \theta$
	3 1 1	3p _y	$\frac{2}{27\sqrt{\pi}a} \left(\frac{Z}{a}\right)^{3/2} \frac{Zr}{a} \left(1 - \frac{Zr}{6a}\right) \exp\left(-\frac{Zr}{3a}\right) \sin \theta \cos \phi$
	3 1 -1	3p _x	$\frac{2}{27\sqrt{\pi}a} \left(\frac{Z}{a}\right)^{3/2} \frac{Zr}{a} \left(1 - \frac{Zr}{6a}\right) \exp\left(-\frac{Zr}{3a}\right) \sin \theta \sin \phi$
	3 2 0	3d _{z²}	$\frac{1}{81\sqrt{6\pi}} \left(\frac{Z}{a}\right)^{3/2} (3 \cos^2 \theta - 1) \left(\frac{Z^2 r^2}{a^2}\right) \exp\left(-\frac{Zr}{3a}\right)$
	3 2 1	3d _{yz}	$\frac{1}{81\sqrt{\pi}} \left(\frac{Z}{a}\right)^{3/2} \left(\frac{Z^2 r^2}{a^2}\right) \exp\left(-\frac{Zr}{3a}\right) \sin \theta \cos \theta \cos \phi$
	3 2 -1	3d _{xz}	$\frac{1}{81\sqrt{\pi}} \left(\frac{Z}{a}\right)^{3/2} \left(\frac{Z^2 r^2}{a^2}\right) \exp\left(-\frac{Zr}{3a}\right) \sin \theta \cos \theta \sin \phi$
	3 2 2	3d _{x²-y²}	$\frac{1}{162\sqrt{\pi}} \left(\frac{Z}{a}\right)^{3/2} \left(\frac{Z^2 r^2}{a^2}\right) \exp\left(-\frac{Zr}{3a}\right) \sin^2 \theta \cos 2\phi$
	3 2 -2	3d _{xy}	$\frac{1}{162\sqrt{\pi}} \left(\frac{Z}{a}\right)^{3/2} \left(\frac{Z^2 r^2}{a^2}\right) \exp\left(-\frac{Zr}{3a}\right) \sin^2 \theta \sin 2\phi$

⁹⁰ state is given by

$$W = \left| \int \psi_0^2 \exp(-iq \cdot r) dV \right| = \left| \int_0^\infty \int_0^\pi \int_0^{2\pi} \psi_0^2 \exp(-iqr \cos \theta) r^2 \sin \theta dr d\theta d\phi \right| \quad (5)$$

Similar formalism is also applicable for projectile nuclei. Using Table 1, we can get the probability of electron to remain in same state (K-, L- and M- shell) after the sudden jolt of respective nuclei by integration of Eq. 5.

The results obtained are following

$$W_{100}^K = \frac{256Z^8}{(a^2q^2 + 4Z^2)^4} \quad (6)$$

$$W_{200}^L = \frac{Z^8 (2a^4q^4 - 3a^2q^2Z^2 + Z^4)^2}{(a^2q^2 + Z^2)^8} \quad (7)$$

$$W_{210}^L = \frac{Z^{12} (Z^2 - 5a^2q^2)^2}{(a^2q^2 + Z^2)^8} \quad (8)$$

$$W_{211}^L = W_{21-1}^L = \frac{4Z^{12}}{(a^2q^2 + Z^2)^6} \quad (9)$$

$$W_{300}^M = \frac{256Z^8 (3a^2q^2 - 4Z^2)^2 (27a^2q^2 - 4Z^2)^2 (243a^4q^4 - 216a^2q^2Z^2 + 16Z^4)^2}{(9a^2q^2 + 4Z^2)^{12}} \quad (10)$$

$$W_{310}^M = \frac{65536Z^{12} (3645a^6q^6 - 3321a^4q^4Z^2 + 648a^2q^2Z^4 - 16Z^6)^2}{(9a^2q^2 + 4Z^2)^{12}} \quad (11)$$

$$W_{311}^M = W_{31-1}^M = \frac{262144Z^{10} (81a^4q^4Z - 27a^2q^2Z^3 + 4Z^5)^2}{(9a^2q^2 + 4Z^2)^{10}} \quad (12)$$

$$W_{320}^M = \frac{65536Z^{14} (1377a^4q^4Z - 312a^2q^2Z^3 + 16Z^5)^2}{(9a^2q^2 + 4Z^2)^{12}} \quad (13)$$

$$W_{321}^M = W_{32-1}^M = \frac{262144Z^{14} (63a^2q^2Z - 4Z^3)^2}{(9a^2q^2 + 4Z^2)^{10}} \quad (14)$$

$$W_{322}^M = W_{32-2}^M = \frac{262144Z^{16}}{(9a^2q^2 + 4Z^2)^8} \quad (15)$$

where W_{nlm}^K , W_{nlm}^L and W_{nlm}^M are the probability that the electron will remain in same shell i.e. K-, L- and M- shell, respectively and a = Bohr radius and Z = atomic number of the projectile or target according to the case. For the

case of Hydrogen atom Eq. 6 reduces to the earlier reported value [14] i.e.

$$W_{100}^K = 1 / \left(1 + \frac{a^2 q^2}{4} \right)^4.$$

Thus the shaking probability is defined by

$$W_{shaking} = 1 - W \quad (16)$$

where W can be replaced by W_{100}^K , $\sum_{2lm} W_{nlm}^L$ or $\sum_{3lm} W_{nlm}^M$ from Eq. 6 -
110 15 to get the shaking probability, $W_{shaking}$, for K-, L- and M- shell electrons respectively.

It is found that for the values of $a.q \ll 1$, shaking probability reduces to 0 whereas for the $a.q \gg 1$ it equals to unity. Interestingly during the fast ion-atom collisions, condition $a.q \gg 1$ is applicable in wide range of recoil energy
115 (starts from keV). Noteworthy that applicability of the condition of suddenness during perturbation requires higher incident energy in the ion-atom collisions than required by the recoil energy of respective nuclei for the shaking. It clearly suggests that once the sudden approximation condition is satisfied it will naturally assured the limiting condition $a.q \gg 1$.

120 4. Conclusion

We have calculated the shaking probabilities accompanying the ion-atom collisions using the hydrogenic wavefunctions for K-, L- and M- shell electrons. It is found that in the limiting case i.e. $a.q \ll 1$, the shaking probability tends to zero, whereas for $a.q \gg 1$ it tends to unity. Interestingly, the condition $a.q$
125 $\gg 1$ holds good even for the low recoil cases (starting from keV/u). During the fast ion-atom collision suddenness of impact can satisfy this condition very well. Thus this study implies that during fast heavy ion-atom collisions, one of the most probable channel of electron transitions is the shaking (shakeup + shakeoff), which occurs due to sudden jolt of projectile/target nuclei in the
130 collisions.

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